MST e-NEWS

September 2011

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Robert Field, MST-6, top and Deniece Korzekwa, MST-16.

Field, Korzekwa named ASM Fellows

Robert Field (Materials Technology: Metallurgy, MST-6) and Deniece Korzekwa (Nuclear Materials Science, MST-16) were recently named Fellows of ASM International, selected by the organization's board of trustees in honor of their distinguished contributions in the field of materials science and engineering. Also selected was Amit Misra (Center for Integrated Nanotechnologies, MPA-CINT).

Field was cited for "applied research of superalloys, intermetallic compounds, and beryllium alloys, dislocation and deformation analysis, and characterization of deformation mechanisms in uranium alloys through excellence in crystallography and electron microscopy."

Korzekwa was cited "For outstanding contributions in the field of casting, fluid flow and solidification modeling of actinide metals, and impact of that research on national security. In further recognition of her tireless mentoring and outreach to our next generation scientists and service to ASM International, especially the Los Alamos Chapter."

Field, the team leader for miscrostructural characterization in MST-6 and the deputy leader of the Materials Design Institute at Los Alamos, received his PhD in metallurgical engineering from the University of Illinois at Urbana/Champaign, specializing in the application of electron microscopy to address materials problems. He joined the Laboratory in 1994. His current research interests are primarily in the area of uranium and its alloys.

Korzekwa, who joined the Laboratory in 1986, is group leader for MST-16. Previously she was the team leader for the Foundry, Machining and Deformation Processing team within MST-6. Korzekwa received a BS in metallurgical engineering from the Colorado School of Mines and a MS in multidisciplinary engineering from Purdue University. Her research interests have focused on a coupled simulation/experimental program incorporating the application of fluid flow and solidification modeling for nuclear material casting processes.

The solicited guidance from Fellows enhances the society's standing as a leading organization for materials with 36,000 members worldwide and provides a unique resource to serve the worldwide community of materials scientists and engineers in the years ahead. The recipients will be honored during a ceremony at the MS&T'11, the Materials Science & Technology 2011 Conference & Exhibition, to be held in October in Columbus, Ohio.

Welch leads online video chat with high school science students

Cynthia Welch (Polymers and Coatings, MST-7) recently participated in an online video chat with the Lincoln Interactive Cutting Edge Science Club. Lincoln Interactive, a leading developer of online-delivered K-12 curriculum, has collaborated with Laboratory staff in connecting students directly with researchers and engineers working at Los Alamos. The chat was planned and moderated by Steve Stringer (Tech Transfer, TT-DO) and Caroline Hardman, Lincoln Interactive's STEM Program Coordinator and two Lincoln interactive science teachers.

The chat focused on Welch's research in the field of polymer science, especially in the area of fuel cell technology. The students, who range from 8th to 12th graders, were curious about all aspects of fuel cell technology, including the level of efficiency a fuel cell can achieve, what fuel cell applications are being developed other than automotive applications, and if fuel cell operations pose any environmental concerns. The students also had several questions relating to Welch's general career experiences as a scientist.

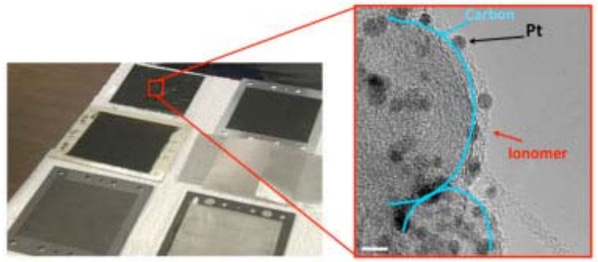
The discussion with Welch was conducted using online software that has video, audio, text chatting, and other interactive components. A week prior, the students prepared for the discussion with their club advisors. The advisors plan the annual program, which includes live chats that introduce the students to a new scientist and a different topic each month. The program, which began in January 2009, is designed to engage students in a deeper exploration of science and technologies being researched and developed at Los Alamos. This unique educational opportunity offers students a look at what it is like to work in various science and technology careers. Students in the program also explore the impact of today's research on the innovations that will drive our global society in the decades to come.

As a result of the success of this event, Welch has been asked by one of her former professors at her undergraduate institution, the University of Southern Mississippi, to hold a similar program for a freshman-level introduction to polymers class next spring.

Last summer Welch was similarly interviewed for Lincoln Interactive's engineering curriculum.

Los Alamos scientists have participated in numerous video interviews that are incorporated directly into accredited science lessons available online, effectively demonstrating for students the real-world application of instructional concepts. The videos, (featuring Welch and 31 other Laboratory scientists) have been published in Lincoln Interactive's Cutting Edge Science courses, which focus on energy science and engineering topics, and are geared to students in high school and middle school.

Technical contact: Cynthia Welch, Steve Stringer



Photos of fuel cell membranes, electrodes, and membrane-electrode assemblies. The electrode is a thin film consisting of carbon-supported catalyst particles and an ionic polymer (or ionomer), as shown in the HR-TEM image (scale bar = 5 nm).

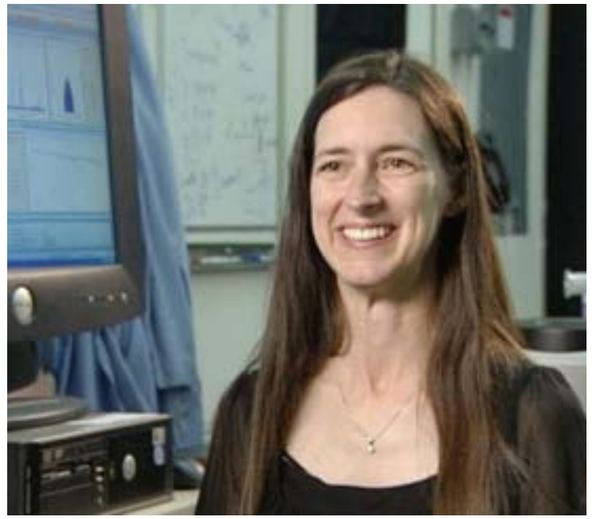


Image of Cynthia Welch during the interview session with Lincoln Interactive.

U and Xe transport in $UO_{2\pm x}$: Density functional theory calculations

Fission gases in uranium dioxide (UO_2) nuclear fuel, of which xenon (Xe) is one of the most prominent, influence fuel performance during both normal and accident reactor conditions. Improved understanding of fission gas behavior may lead to improved reactor operation via high fidelity models of fission gas transport in fuel performance simulation codes.

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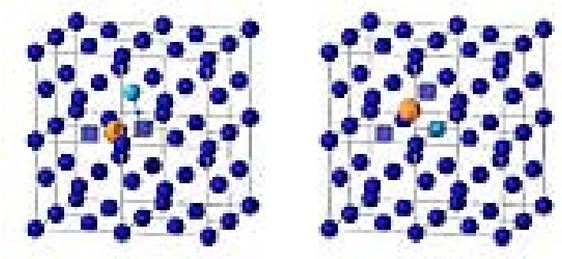
Calculations… Using density functional theory calculations, Los Alamos scientists have calculated the activation energies for Xe diffusion in $UO_{2\pm x}$ as well as the closely related activation energies for uranium (U) diffusion, thus providing new insights into the mechanisms by which species transport occurs in UO_2.

Their results show that Xe transport occurs by binding a uranium vacancy to the stable Xe trap sites in the UO_2 lattice; these clusters then migrate according to a vacancy-mediated mechanism. Unlike typical vacancy diffusion, the vacancy and Xe atom remain bound during the migration process. Calculating the corresponding activation energy for U transport also requires us to consider defect cluster formation, in particular for cases where excess concentrations of defects are present such as under irradiation in reactor environments. For example, their calculations reveal that the experimental migration barrier refers to diffusion of clusters containing two U vacancies. In order to reach accurate predictions for both Xe and U transport, it is essential to treat the charge compensation for defects in $UO_{2\pm x}$ in a consistent way.



Schematic illustration of Xe diffusion via a vacancy mediated mechanism. For simplicity O atoms are omitted and only U atoms are shown. Xe atoms are shown in yellow, U in blue, and vacancies are represented by squares. The highlighted U atom can migrate into one of the cluster vacancies, thus giving rise to net Xe diffusion. The right-hand figure is equivalent to the defect cluster in the left-hand figure, but with the highlighted U atom translated from its original position into the nearest neighbor vacancy site along the [1/2 01/2] lattice vector.

Reference: "U and Xe transport in $UO_{2\pm x}$: Density functional theory calculations," by David Andersson, Blas Uberuaga, Panjaj Nerikar, Chris Stanek (all Structure/Property Relations, MST-8), and Cetin Unal (Decision Applications, D-DO), accepted for publication in *Physical Review B* as an Editor's Suggestion.

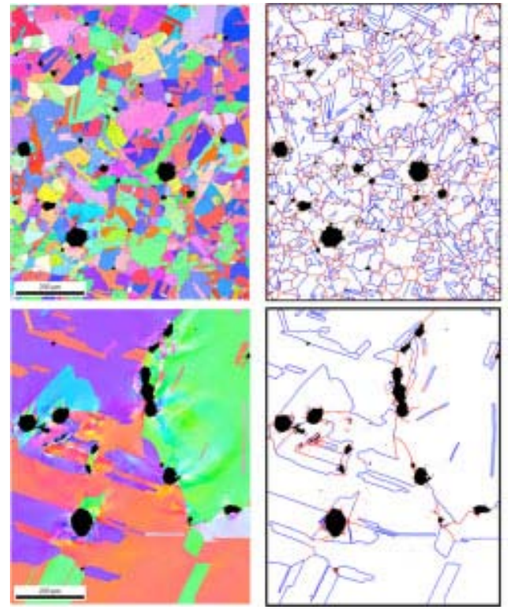
Work at Los Alamos National Laboratory was funded by the DOE Nuclear Energy Fuel Cycle Research and Development Campaign, Nuclear Energy Advanced Modeling and Simulation Program, Fuels Integrated Performance and Safety Code project under the AFCI Modeling and Simulation program.

Technical contact: David Andersson

Effects of grain size and boundary structure on the dynamic tensile response of copper

As part of Los Alamos's role in evaluating materials performance in extreme environments, Laboratory researchers have conducted shock experiments to examine the effect of grain boundary characteristics on the dynamic tensile response of copper samples.

Their research, accepted for publication in the *Journal of Applied Physics*, revealed that damage in these extreme conditions occurs at locations determined by the structure of the grain boundaries. This deterministic behavior has implications across a wide range of applications for industries such as aerospace, automotive, and defense.



EBSD maps (a) Orientation (color represents a specific orientation of a given grain according to the triangle on the right), (b) grain boundary (colors are based on the boundary structure; voids are preferentially located on red-colored grain boundaries).

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Grain size... To examine the fundamental mechanisms of damage evolution (i.e. void nucleation, growth, and coalescence), the researchers dynamically loaded high purity copper specimens in the gas gun facilities in Shock and Detonation Physics, WX-9.

Care was taken to load these specimens in such a way as to only incipiently damage these specimens rather than completely fail or fracture them. All specimens were carefully soft recovered after dynamic loading and characterized using the electron microscopy facilities in MST-6.

Prior to dynamic loading, the high purity copper specimens had a known defect distribution, i.e.: grain boundary density/distribution (grain size). Four different microstructures were studied. The differences in the damage evolution of the dynamically loaded specimens were rationalized in terms of the initial microstructural characteristics. Characterization of the resultant damage was performed via optical and electron backscatter diffraction analyses (EBSD), (see figure).

Reference: "Effects of grain size and boundary structure on the dynamic tensile response of copper" by J. Pablo Escobedo, Ricardo Lebensohn and Ellen Cerreta (MST-8); Brian Patterson (MST-7); Darcie Dennis-Koller (WX-9), Ben Hansen and Curt Bronkhorst (Fluid Dynamics and Solid Mechanics, T-3); and Davis Tonks (Materials and Physical Data, XCP-5), *Journal of Applied Physics* **110** (in press).

The Laboratory Directed Research and Development program funded the research.

Technical contact: J. Pablo Escobedo

Using advanced characterization techniques to probe damage evolution

Additional contributors to the research featured in "Using advanced characterization techniques to probe damage evolution," which appeared in last month's *MST e-news*, include Chris Chen and Denny Guidry (both MST-6).

Celebrating service

Congratulations to the following MST employees celebrating service anniversaries this month:

Gerald Rivera, MST-7	25 years
Randall Randolph, MST-7	25 years
Carlos Tome, MST-8	15 years
Michael Ramos, MST-16	15 years
Ming Tang, MST-8	5 years
Nickolaus Smith, MST-7	5 years
Jian Wang, MST-8	5 years

HeadsUP!

Seasonal flu vaccine available through local pharmacies

The 2011 seasonal flu vaccine is available now from area pharmacies, clinics, and personal medical providers. The Occupational Medicine Clinic will not be providing the flu vaccine onsite except for those Laboratory workers who receive the vaccine as part of their medical surveillance program. A list indicating the nearly 200 pharmacies in New Mexico contracted by Blue Cross Blue Shield of New Mexico to provide the seasonal flu vaccine at no out-of-pocket charge to individuals covered by the BC/BS health plan is located at int.lanl.gov/news/newsbulletin/pdf/vaccine_network_list_092810.pdf. Call pharmacies first to find out when the flu vaccine will be offered, as hours may vary among sites.

LANL Traffic Webcam

The LANL Traffic webcam provides an eastbound view of Diamond Drive and West Jemez Road conditions and allows LANL employees to better plan their route during inclement weather or in the case of an emergency. Please see int.lanl.gov/projects/webcam/.

Vehicle weight limit to be enforced at parking structures

The Protective Force will ticket vehicles that exceed the maximum posted weight limits in the parking structures at Technical Area 3. Drivers whose vehicles exceed 6,000 pounds must park in open (surface) lots, such as near the park-and-ride lot east of Diamond Drive at East Jemez Road (the truck route). Gross vehicle weights are usually found on the inside of the driver's-side door frames. Visit int.lanl.gov/security/physical/parking_structures.shtml for more information.

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